Modulated pair condensate of p-orbital ultracold fermions

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(Dated: September 16, 2010)

We show that an interesting of pairing occurs for spin-imbalanced Fermi gases under a specific experimental condition—the spin up and spin down Fermi levels lying within the p_x and s orbital bands of an optical lattice, respectively. The pairs condense at a finite momentum equal to the sum of the two Fermi momenta of spin up and spin down fermions and form a p-orbital pair condensate. This $2k_F$ momentum dependence has been seen before in the spin- and charge- density waves, but it differs from the usual p-wave superfluids such as ^{3}He, where the orbital symmetry refers to the relative motion within each pair. Our conclusion is based on the density matrix renormalization group analysis for the one-dimensional (1D) system and mean-field theory for the quasi-1D system. The phase diagram of the quasi-1D system is calculated, showing that the p-orbital pair condensate occurs in a wide range of fillings. In the strongly attractive limit, the system realizes an unconventional BEC beyond Feynman's no-node theorem. The possible experimental signatures of this phase in molecule projection experiment are discussed.

PACS numbers: 03.75.Ss, 71.10.Fd, 37.10.Jk, 05.30.Fk

I. INTRODUCTION

Pairing with mismatched Fermi surfaces has long fascinated researchers in the fields of heavy fermion and organic superconductors, color superconductivity in quark matter [1], and, most recently, ultracold Fermi gases with spin imbalance [2–5]. In a classic two-component model for superconductivity, the mismatch arises from the spin polarization of fermions in the same energy band. Its effect was predicted to produce intriguing, unconventional superfluids such as the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) [6, 7], deformed Fermi surface [8, 9], and breached pair phases [10, 11]. The limiting case of large spin imbalance was also studied to explore the formation of Fermi polarons [12]. In parallel, the behavior of particles in the higher orbital bands of optical lattices, due to large filling factors, thermal excitations or strong interactions, is widely studied for novel orbital orderings of both bosons [13–15] and fermions [16, 17] with repulsive interactions. Recently, interband pairing of unpolarized fermions was shown theoretically to give rise to Cooper pair density waves [18].

In this article, we report a fermion pairing phase resulting from the interplay of Fermi surface mismatch and p-orbital band physics. In such a phase, the pair condensate wave function is spatially modulated and has a p-wave symmetry. This phase arises in an attractive two-component Fermi gas on anisotropic optical lattices under a previously unexplored condition of spin imbalance. Namely the majority ($\uparrow$) spin and the minority ($\downarrow$) spin occupy up to Fermi levels lying in the p_x and s bands, respectively. We show that pairings take place near the respective Fermi surfaces of the spin $\uparrow$ fermions in p_x band and $\downarrow$ fermions in s band. This induces a modu-

lated p-orbital pair condensate that differs from the usual p-wave superfluids such as ^{3}He. The state requires only an on-site isotropic contact interaction and the pair is a spin singlet, while the ^{3}He p-wave superconductivity has to involve anisotropic interaction and spin triplet. The modulation wave vector of the order parameter is $Q \approx k_{F\uparrow} + k_{F\downarrow}$, where $k_{F\uparrow}$, $k_{F\downarrow}$ are Fermi momenta for spin $\uparrow$ and $\downarrow$ species, respectively. This $2k_F$ momentum dependence is an unprecedented signature in superfluids other than the spin- and charge- density waves. In the strongly attractive limit, tightly bounded pairs condense at finite momentum Q, which realizes an unconventional Bose-Einstein condensate beyond Feynman's no-node theorem [13–15, 19, 20].

II. MODEL

The system under consideration is at zero temperature and consists of two-component fermions in a three-dimensional (3D) cubic optical lattice with lattice constant a, described by the Hamiltonian

$$H = \sum_\sigma \int d^3\mathbf{x}\, \psi_\sigma^\dagger(\mathbf{x})[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) - \mu_\sigma]\psi_\sigma(\mathbf{x})$$
$$+ g \int d^3\mathbf{x}\, \psi_\uparrow^\dagger(\mathbf{x})\psi_\downarrow^\dagger(\mathbf{x})\psi_\downarrow(\mathbf{x})\psi_\uparrow(\mathbf{x}). \quad (1)$$

Here $\psi_\sigma(\mathbf{x})$ is the fermionic field operator at $\mathbf{x}$ with spin $\sigma = \uparrow, \downarrow$, $V(\mathbf{x})$ is the lattice potential, μ_σ is the chemical potential for spin σ fermions, and $g < 0$ is the contact attraction which can be tuned by the Feshbach resonance. In particular, we consider the case where the lattice potential in the x (parallel) direction is much weaker than

the other two (transverse) directions, so the system behaves quasi-one-dimensionally.

We expand $\psi_\sigma(\mathbf{x}) = \sum_{n\mathbf{r}} \phi_n(\mathbf{x}-\mathbf{r})c_{n\mathbf{r}}$, where $\phi_n(\mathbf{x}-\mathbf{r})$ is the nth band Wannier function at lattice site $\mathbf{r}$ with $c_{n\mathbf{r}}$ the annihilation operator in Wannier basis. As a result, we obtain the usual attractive Hubbard model with nearest-neighbor hopping between ith site with orbital band α and jth site with orbital band β

$$t_{\alpha\beta} = -\int d^3\mathbf{x}\phi_\alpha^*(\mathbf{x}-\mathbf{r}_i)\left[-\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{x})\right]\phi_\beta(\mathbf{x}-\mathbf{r}_j) \quad (2)$$

and on-site attraction between orbitals

$$U_{\alpha\beta\gamma\eta} = g\int d^3\mathbf{x}\phi_\alpha^*(\mathbf{x}-\mathbf{r}_i)\phi_\beta^*(\mathbf{x}-\mathbf{r}_i)\phi_\gamma(\mathbf{x}-\mathbf{r}_i)\phi_\eta(\mathbf{x}-\mathbf{r}_i). \quad (3)$$

The lowest two energy bands are the s and p_x band (the p_y and p_z band are much higher in energy because of tighter confinement in the transverse directions). For brevity the p_x band is simply called p band in the following. By filling fermions with spin $\uparrow$ to the p band and spin $\downarrow$ to the s band, the Hamiltonian becomes

$$H_{sp} = -\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}(t_s^\parallel S_\mathbf{r}^\dagger S_{\mathbf{r}'} - t_p^\parallel P_\mathbf{r}^\dagger P_{\mathbf{r}'} + h.c.) - \mu_s\sum_\mathbf{r}n_\mathbf{r}^s$$
$$- \sum_{\langle\mathbf{r},\mathbf{r}''\rangle}(t_s^\perp S_\mathbf{r}^\dagger S_{\mathbf{r}''} + t_p^\perp P_\mathbf{r}^\dagger P_{\mathbf{r}''} + h.c.) - \mu_p\sum_\mathbf{r}n_\mathbf{r}^p$$
$$+ \omega_b\sum_\mathbf{r}n_\mathbf{r}^p + U_{sp}\sum_\mathbf{r}n_\mathbf{r}^s n_\mathbf{r}^p. \quad (4)$$

Here, $\langle\mathbf{r},\mathbf{r}'\rangle$ and $\langle\mathbf{r},\mathbf{r}''\rangle$ denote the nearest neighboring lattice sites in parallel and transverse directions. $t_s^\parallel$ and $t_p^\parallel$ are the hopping amplitudes along the parallel direction for the s- and p-band fermions respectively, while $t_s^\perp = t_p^\perp = t^\perp$ are the hopping amplitudes in transverse directions. $S_\mathbf{r}$ ($P_\mathbf{r}$) is the annihilation operator at lattice site $\mathbf{r}$ for s-band $\downarrow$ (p-band $\uparrow$) fermions. $n_\mathbf{r}^s = S_\mathbf{r}^\dagger S_\mathbf{r}, n_\mathbf{r}^p = P_\mathbf{r}^\dagger P_\mathbf{r}$ are the number operators, and μ_s, μ_p are the corresponding chemical potentials. U_{sp} is the attractive on-site interaction between s- and p-band fermions and can be tuned by changing the scattering length using Feshbach resonance. ω_b is related to the band gap. In the tight binding region we assume $\omega_b \gg |U_{sp}|$, and consequently the s-band fully filled spin $\uparrow$ fermions are dynamically inert and not included in the H_{sp}.

III. DMRG CALCULATION FOR 1D CASE

First we consider the pairing problem in the simplest case of 1D ($t^\perp = 0$), which is schematically shown in Fig. 1(a). The two relevant Fermi momenta are $k_{F\downarrow}$ (for s-band $\downarrow$ fermions) and $k_{F\uparrow}$ (for p-band $\uparrow$ fermions). From a weak coupling point of view, to pair fermions of opposite spin near their respective Fermi surfaces, the
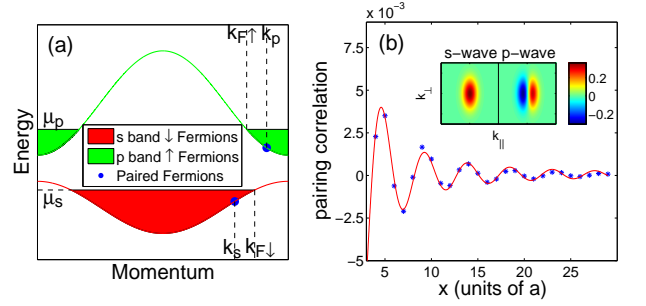

FIG. 1. (Color online) (a) A schematic illustration showing the pairing between s- and p-band fermions. The s band is also fully occupied with $\uparrow$ fermions (not shown). (b) The spatial variation of the pairing correlation $C(x)$ for $N_s = 49$, $N_p = 15$ according to DMRG. The blue scatters are the DMRG result and the solid line is the fitting using function $a\cos(qx+b)/x^\eta + c$. The inset in (b) shows the s- and p-wave Wannier functions in momentum space, which are elongated in the transverse direction (in real space they are compressed in transverse direction). The s-wave Wannier function has even parity while the p-wave Wannier function has odd parity.

Cooper pairs have to carry finite center-of-mass momentum (CMM) due to Fermi surface mismatch. Furthermore, in order for all Cooper pairs to have roughly the same CMM, the only choice is to pair fermions of opposite chirality. Note that the dispersion of p band is inverted with respect to the s band, so pairing occurs between fermions with momenta of the same sign but opposite group velocities. These elementary considerations show that the CMM of the pair should be approximately the sum of two Fermi momenta,

$$Q \approx k_{F\uparrow} + k_{F\downarrow}. \quad (5)$$

This result differs from that of the usual one-dimensional spin imbalanced fermions within the same band, where the FFLO pair momentum is the difference, $Q \approx |k_{F\uparrow} - k_{F\downarrow}|$, as found in a two-leg-ladder system [21].

Mean-field theory and weak coupling consideration can provide only a qualitative picture for 1D problems. To unambiguously identify the nature of the ground state, we use density matrix renormalization group (DMRG) to compute the pair correlation function. In the numerical calculations, we used parameters $t_s^\parallel = 1$ as the unit of energy, $t_p^\parallel = 8$, $\mu_s = 1.7$, $\mu_p - \omega_b = -11$, in which the ratio between t_s and t_p is chosen according to typical tight-binding bandwidth ratio. U_{sp} is tunable with Feshbach resonance and in the following calculation we will focus on $U_{sp} = -9$ [22]. The truncation error is controlled in the order of 10^{-7} or less. Equation (5) predicts $Q \approx k_{F\uparrow} + k_{F\downarrow} = 0.435\pi/a$. Figure 1(b) shows the pairing correlation function in real space $C_{ij} = \langle S_i^\dagger P_i^\dagger P_j S_j\rangle$ as a function of $x = |i-j|$ for a chain of $N = 60$ sites with open boundary condition, where the indices i and j are real space positions. Since the system only has algebraic order, $C(x)$ decays with x according to a power law. On

top of this, however, there is also an obvious oscillation. A curve fit with formula $C(x) = a\cos(qx + b)/x^\eta + c$, shown in Fig. 1(b), yields a period of $q = 0.438\pi/a$, which is in good agreement with the wave number given by Eq. (5) before. The Fourier transform of the pair correlation function

$$C_q = \frac{1}{N}\sum_{i,j}e^{iq(i-j)}C_{ij} \qquad (6)$$

is peaked at $q = 0.426\pi/a$ (to be plotted in Sec. VI). These features of the pair correlation function are the signature of the existence of the $2k_F$ CMM pairing in our system [23, 24].

IV. MEANFIELD ANALYSIS FOR QUASI 1D CASE

Now we move on to the quasi-1D system where a weak transverse hopping $t^\perp \ll t^\parallel$ is added. We carry out a mean-field analysis of Hamiltonian H_{sp} by introducing the s-p pairing order parameter

$$\Delta_{\mathbf{r}} = U_{sp}\langle S_{\mathbf{r}}P_{\mathbf{r}}\rangle, \qquad (7)$$

where $\langle...\rangle$ means the ground-state expectation value. Two different trial ground states are investigated, the exponential wave $\Delta_{\mathbf{r}} = \Delta e^{i\mathbf{Q}\cdot\mathbf{r}}$, which is analogous to the Fulde-Ferrell phase and the cosine wave $\Delta_{\mathbf{r}} = \Delta\cos\mathbf{Q}\cdot\mathbf{r}$, which is analogous to the Larkin-Ovchinnikov phase. $\mathbf{Q}$ and Δ are determined self-consistently by minimization of ground-state free energy $\langle H_{sp}\rangle$. Transverse hopping introduces a small Fermi surface curvature and spoils the perfect nesting condition as in the pure 1D problem above. However, the curvature is small for weak $t^\perp$. Thus, we expect $\mathbf{Q}$ pointing almost along the parallel direction, $\mathbf{Q} = Q(1,0,0)$, in order to maximize the phase space of pairing.

The mean-field Hamiltonian for the exponential wave can be diagonalized in momentum space by standard procedure. We get the ground state energy

$$\langle H_{sp}\rangle = \sum_{\mathbf{k},\gamma=\pm}\Theta(-\lambda_{\mathbf{k}}^{(\gamma)})\lambda_{\mathbf{k}}^{(\gamma)} + \sum_{\mathbf{k}}\xi_{\mathbf{k}}^p - \frac{N^3\Delta^2}{U_{sp}} \quad (8)$$

with the self-consistent gap equation for Δ

$$1 = \frac{U_{sp}}{N^3}\sum_{\mathbf{k}}\frac{\Theta(-\lambda_{\mathbf{k}}^{(+)}) - \Theta(-\lambda_{\mathbf{k}}^{(-)})}{\sqrt{4\Delta^2 + (\xi_{\mathbf{k}}^s + \xi_{\mathbf{Q}-\mathbf{k}}^p)^2}}. \qquad (9)$$

Here, $\mathbf{k}$ is lattice momentum, N^3 is the total number of sites, Θ is a step function, and $\lambda_{\mathbf{k}}^{(\pm)} = \frac{1}{2}[\xi_{\mathbf{k}}^s - \xi_{\mathbf{Q}-\mathbf{k}}^p \pm \sqrt{4\Delta^2 + (\xi_{\mathbf{k}}^s + \xi_{\mathbf{Q}-\mathbf{k}}^p)^2}]$ is the eigenenergy of the Bogoliubov quasiparticles. As evident from these formulas, the pairing occurs between an s-band fermion of momentum $\mathbf{k}$ and a p-band fermion of momentum $\mathbf{Q} - \mathbf{k}$ with dispersion $\xi_{\mathbf{k}}^s = -2t_s^\parallel\cos k_x a - 2t^\perp\cos k_y a - 2t^\perp\cos k_z a - \mu_s$

and $\xi_{\mathbf{k}}^p = 2t_p^\parallel\cos k_x a - 2t^\perp\cos k_y a - 2t^\perp\cos k_z a - \mu_p + \omega_b$, respectively.

The cosine wave is spatially inhomogeneous. A full mean-field analysis requires solving the Bogoliubov-de Gennes equation to determine the gap profile self-consistently. Here we are interested only in computing the free energy for the ansatz $\Delta_{\mathbf{r}} = \Delta\cos\mathbf{Q}\cdot\mathbf{r}$ to compare with the exponential wave case. Thus, it is sufficient to numerically diagonalize the full Hamiltonian Eq. (4) for a finite size lattice. We introduce a vector of dimension $2N$

$$\alpha_{k_y k_z}^\dagger = (S_{k_x^1 k_y k_z}^\dagger...S_{k_x^N k_y k_z}^\dagger, P_{k_x^1,-k_y,-k_z}...P_{k_x^N,-k_y,-k_z}), \qquad (10)$$

where $k_x^n = 2\pi n/Na$ is the discrete momentum in the x direction. The components of α obey anticommutation relation $\{\alpha_{k_y k_z}^{\dagger(m_1)},\alpha_{k_y k_z}^{(m_2)}\} = \delta_{m_1 m_2}$, where m_1, m_2 labels the corresponding operator component of α. The Hamiltonian takes the compact form $H_{sp} = \sum_{k_y k_z}\alpha_{k_y k_z}^\dagger\mathcal{H}_{k_y k_z}\alpha_{k_y k_z} + \sum_{\mathbf{k}}\xi_{\mathbf{k}}^p - (1 + \delta_{Q,-Q})N^3\Delta^2/2U_{sp}$. Since $\mathcal{H}_{k_y k_z}$ is real and symmetric, it can be diagonalized by an orthogonal transformation $\alpha_{k_y k_z} = \mathcal{D}_{k_y k_z}\beta_{k_y k_z}$ to yield $2N$ eigenvalues $E_{k_y k_z}^l$. The new operators $\beta_{k_y k_z}$ automatically obey the fermionic anticommutation relationship $\{\beta_{k_y k_z}^{\dagger(m_1)},\beta_{k_y k_z}^{(m_2)}\} = \delta_{m_1 m_2}$. We get the ground state energy,

$$\langle H_{sp}\rangle = \sum_{k_y,k_z}\sum_{l=1}^{2N}E_{k_y k_z}^l\Theta(-E_{k_y k_z}^l) + \sum_{\mathbf{k}}\xi_{\mathbf{k}}^p$$
$$- \frac{N^3\Delta^2}{2U_{sp}}(1 + \delta_{-Q,Q}), \qquad (11)$$

and the gap equation,

$$\Delta = \frac{2U_{sp}}{N^3(1 + \delta_{-Q,Q})}\sum_{\mathbf{k}}\sum_l\mathcal{D}_{k_y k_z}^{m_1,l}\mathcal{D}_{k_y k_z}^{m_1',l}\Theta(E_{k_y k_z}^l). \quad (12)$$

Here, l labels the eigenenergy, and m_1, m_1' labels the matrix elements corresponding to the original S, P operators in the gap equation.

The parameters used in the mean-field calculations are the same as in the 1D case with small $t^\perp$'s added, and we still expect that the order parameter has the momentum around $0.435\pi/a$ as before. By self-consistently solving for Q and Δ, in the case $t^\perp = 0.05$, the ground state is the cosine wave phase with $Q = 0.433\pi/a$ and $\Delta = 0.822$. The ground state energy per site is -2.5927, lower than the noninteracting value -2.5896. When $t^\perp = 0.1$, the ground state is also the cosine wave phase with $Q = 0.433\pi/a$ and $\Delta = 0.542$. The ground state energy per site is -2.5955, lower than the noninteracting value -2.5949. These results confirm that (i) the cosine wave state has lower energy than the exponential wave state, (ii) the order parameter has the momentum close to the prediction of Eq. (5), and (iii) larger transverse hopping tends to destroy the p-orbital pair condensate since
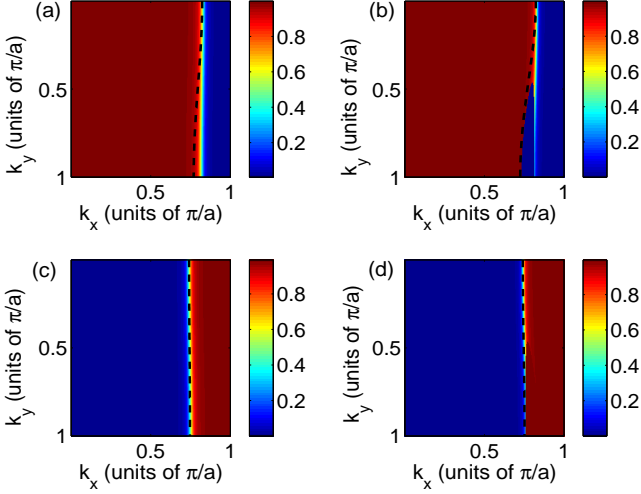
FIG. 2. (Color online) The occupation of s and p band within the paired state for different transverse hopping $t_\perp$. Only the first quadrant of the Brillouin zone in the $k_x - k_y$ plane is shown, $k_z = \pi/a$. The black dashed lines indicate the "bare" Fermi surfaces for corresponding noninteracting fermions ($U_{sp} = 0$). (a) $\langle S_{\mathbf{k}}^\dagger S_{\mathbf{k}} \rangle$ for $t^\perp = 0.05$; (b) $\langle S_{\mathbf{k}}^\dagger S_{\mathbf{k}} \rangle$ for $t^\perp = 0.1$; (c) $\langle P_{\mathbf{k}}^\dagger P_{\mathbf{k}} \rangle$ for $t^\perp = 0.05$; (d) $\langle P_{\mathbf{k}}^\dagger P_{\mathbf{k}} \rangle$ for $t^\perp = 0.1$.

the energy gain for larger transverse hopping is much smaller than for smaller transverse hopping.

An interesting feature of the p-orbital pair condensate in quasi-1D is the possible existence of Fermi surfaces with gapless energy spectrum. We monitor the fermion occupation number, i.e. $\langle S_{\mathbf{k}}^\dagger S_{\mathbf{k}} \rangle$ and $\langle P_{\mathbf{k}}^\dagger P_{\mathbf{k}} \rangle$ for increasing transverse hopping. The results are shown in Fig. 2. For small $t^\perp$, they take the usual BCS form and vary smoothly from 1 (red) to 0 (blue) across the bare Fermi surface (with interaction turned off), as shown in Figs. 2(a) and 2(c) for $t^\perp = 0.05$. For larger transverse hopping, sharp Fermi surfaces characterized by a sudden jump in $\langle S_{\mathbf{k}}^\dagger S_{\mathbf{k}} \rangle$ and $\langle P_{\mathbf{k}}^\dagger P_{\mathbf{k}} \rangle$ appear. This is clearly shown in Figs. 2(b) and 2(d) for $t^\perp = 0.1$ as the occupation number changes discontinuously from 1 (red) to 0 (blue). It can be understood qualitatively as follows. As $t^\perp$ increases, the original Fermi surfaces acquire a larger curvature in the transverse directions and the pairing condition in Eq. (5) cannot be satisfied everywhere anymore. Therefore in some regions fermions are not paired and Fermi surfaces survive. One should also note that the calculation is based on the assumption that $t^\perp \ll t^\parallel$, which predicts that $\mathbf{Q}$ is in the parallel direction. This prediction should fail as $t^\perp$ increases beyond certain critical values.

V. PHASE DIAGRAM

Now, we systematically explore the phases of our system for general band filling and spin imbalance. Since we have s- and p- bands with different bandwidths, we
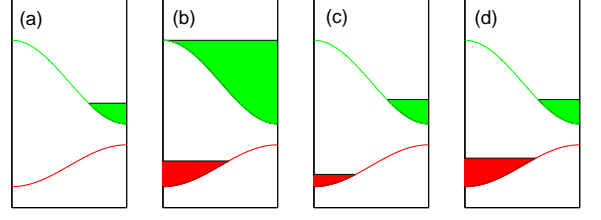

FIG. 3. (Color online) Band occupation for the four possible phases in the system. The band colored in red represents the s band occupied by spin $\downarrow$ fermions and the band colored in green represents the p band occupied by $\uparrow$ fermions. The spin $\uparrow$ fermions in the s band are not shown since they are inert. (a) Normal phase I (N1) with one band empty and the other partially filled. (b) Normal phase II (N2) with one band fully filled and the other partially filled. (c) Commensurate p-orbital pair condensate (CpPC) with both bands partially filled. The occupation numbers are the same. (d) Incommensurate p-orbital pair condensate (IpPC) with both bands partially filled. The occupation numbers are different.

introduce two dimensionless quantities for the chemical potentials μ_s and μ_p

$$\tilde{\mu}_s = \frac{\mu_s}{2t_s} = \frac{\mu_s}{2},$$
$$\tilde{\mu}_p = \frac{\mu_p - \omega_b}{2t_p} = \frac{\mu_p - \omega_b}{16}. \qquad (13)$$

Thus, for a non-interacting system, $-1 < \tilde{\mu}_s, \tilde{\mu}_p < 1$ control the filling for the s and p-band fermions respectively. We then define the quantities

$$\mu = \frac{\tilde{\mu}_s + \tilde{\mu}_p}{2},$$
$$h = \frac{\tilde{\mu}_s - \tilde{\mu}_p}{2}, \qquad (14)$$

as the parameters controlling the average filling and polarization in the phase diagram. The phase at $-\mu, -h$ is the same as the state at μ, h, since the transformation $\mu, h \rightarrow -\mu, -h$ gives $\mu_s, \mu_p \rightarrow -\mu_s, -\mu_p$, and the mean-field Hamiltonian with μ_s, μ_p is identical to Hamiltonian with $-\mu_s, -\mu_p$ via a particle-hole transformation up to a constant.

We have four possible phases in such a system as shown in Fig. 3. As before, we ignored the inert fully filled s band of spin $\uparrow$ fermions. We consider the p band of spin $\uparrow$ fermions and s band of spin $\downarrow$ fermions. When one of these two bands is empty and the other is filled, the pairing does not happen and we call it normal phase I (N1) as in Fig. 3(a). When one of these two bands is fully filled and the other is partially filled, the pairing also does not happen since the fully filled band is inert. We call it normal phase II (N2) as in Fig. 3(b). When both of them are partially filled, fermions near Fermi surfaces from the two bands will be paired and the system is in superfluid phases as shown in Figs. 3(c) and 3(d). In the superfluid regime, when h is small, the pairing momentum prefers $Q = \pi/a$ and we call it commensurate p-orbital pair condensate (CpPC). It is a special case of the p-orbital pair

condensate, where the occupation numbers of s-band spin $\downarrow$ fermions and p-band spin $\uparrow$ fermions are the same. It is similar to the conventional unpolarized pairing (BCS), where the spin $\uparrow$ fermions and spin $\downarrow$ fermions have the same population. However, in BCS pairing the CMM of the pair has the property $Q = 0$, while here $Q = \pi/a$. To understand the momentum π/a preference, note that in conventional BCS case, the two species of fermions have the same energy spectrum and the pairing is between two fermions with opposite momenta, which leads to the CMM of pair $Q = 0$. Here, the structure of energy spectrum of p band is different from s band. The equal occupation numbers mean $k_{F\uparrow} = \pi/a - k_{F\downarrow}$, which gives rise to $Q = k_{F\uparrow} + k_{F\downarrow} = \pi/a$, as shown in Fig. 3(c). At last, when h is large, the pairing momentum stays at a general $Q \approx k_{F\uparrow} + k_{F\downarrow}$ and the occupation number for the two species of fermions differ. We call it incommensurate p-orbital pair condensate (IpPC) as shown in Fig. 3(d).

To determine the phases, we minimize the free energy as a function of the pairing amplitude Δ and pairing momentum Q by mean-field analysis using the cosine wave function as outlined in the previous section. When the minimum is realized at $\Delta = 0$, it is normal phase. When Δ is finite, there are two possibilities. When $Q = \pi/a$, it is CpPC. When $Q \neq \pi/a$, it is IpPC. For the transition between superfluid and normal phase, and the transition between CpPC and IpPC, the behaviors of free energy show that the phase transitions are first order in a lattice system. Between the superfluid and normal phases, near the phase transition, Δ changes suddenly from 0 to finite, and the free energy shows two local minima at $\Delta = 0$ and $\Delta \neq 0$. Between CpPC and IpPC, the pairing momentum changes from $Q = \pi/a$ to $Q \neq \pi/a$ discontinuously, and the free energy as a function of Q also has two local minima at $Q = \pi/a$ and $Q \neq \pi/a$. Thus, they are first-order phase transitions according to our mean field analysis. Therefore, we can determine the phase boundaries between normal phase and superfluid phase by monitoring Δ changing from zero to finite. We can also monitor Q changing from $Q = \pi/a$ to $Q \neq \pi/a$ to determine the phase boundaries between CpPC and IpPC.

In Fig. 4, we present a phase diagram for $t^{\perp} = 0.05$. The x's in Fig. 4 show the data points for the phase boundary obtained from the numerical procedure, and by connecting them we get the phase boundaries. An illustrative physical understanding about this phase diagram is as follows. In Fig. 4, when chemical potential difference h is small and the two bands are still partially filled to ensure the pairing, the system tends to stay in CpPC where $Q = \pi/a$. It is similar to the conventional BCS superfluid case. As h becomes larger, as long as the average filling μ is not too large or small and the two bands are still both partially filled, the pairing persists despite the spin imbalance and the system is in IpPC. If μ gets more and more negative, the average filling becomes smaller and smaller, and at certain μ, h, p band of spin $\uparrow$ fermions will be empty and the system will be-
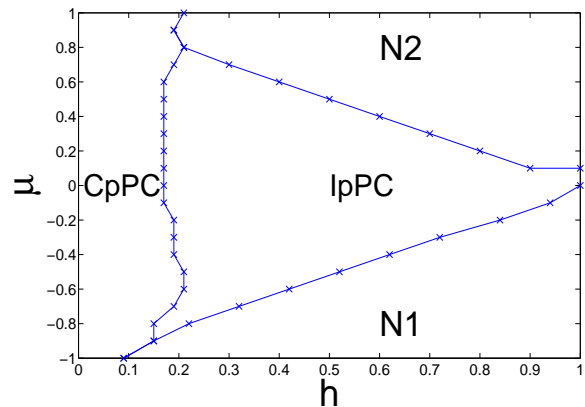

FIG. 4. (Color online) The phase diagram of the p-orbital pair condensate for $t^{\perp} = 0.05$. μ and h are defined in the main text. CpPC: the s band of spin $\downarrow$ fermions and the p band of spin $\uparrow$ fermions have the same occupation numbers. IpPC: the s band of spin $\downarrow$ fermions and the p band of spin $\uparrow$ fermions have different occupation numbers. N1 with the p band of spin $\uparrow$ fermions empty and the s band of spin $\downarrow$ fermions partially filled. N2 with the p band of spin $\uparrow$ fermions partially filled and the s band of spin $\downarrow$ fermions fully filled.

come N1 without pairing. Similarly, when μ is large and positive, the average filling is very high and at certain μ, h, the s band of spin $\downarrow$ fermions will be fully occupied, and the system becomes N2 without pairing. The almost straight phase boundaries in Fig. 4 between IpPC and normal phases indicate that these phase transitions are due to the change of band occupation as empty $\leftrightarrow$ partially filled $\leftrightarrow$ fully filled. In Fig. 4, the phase boundary between IpPC and N1 corresponds to the critical condition that the s band of spin $\downarrow$ fermions is partially filled while the p band of spin $\uparrow$ fermion becomes empty, and the almost straight phase boundary corresponds to the condition that $\tilde{\mu}_p = \mu - h = -1$ (but, as before, this is only an approximate argument due to the presence of interaction). Similarly, the almost straight phase boundary between IpPC and N2 corresponds to the condition that the s band of spin $\downarrow$ fermions becomes fully filled, while the p band of spin $\uparrow$ fermions is partially filled, or $\tilde{\mu}_s = \mu + h = 1$. All the phase transition lines in Fig. 4 are mean field results, and these straight lines are expected to be corrected by quantum critical fluctuations. The phase diagram shows that the p-orbital pair condensate happens in large parameter regimes and is closely related to the band and orbital properties in the optical lattice systems.

VI. SIGNATURE OF THE p-ORBITAL PAIR CONDENSATE IN MOLECULE PROJECTION EXPERIMENT

The p-orbital pair condensate phase can inspire important experimental signatures for finite momentum condensation of bosonic molecules in higher orbital bands.
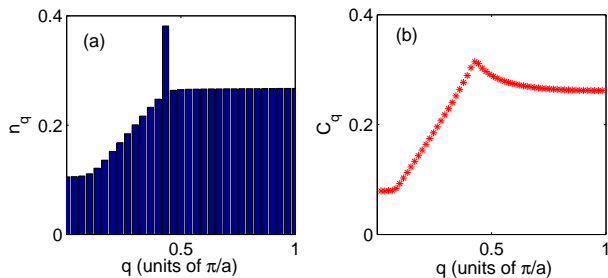
FIG. 5. (Color online) (a) The momentum distribution function n_q of projected molecules for a quasi-1D system with $t^\perp = 0.05$ (all other parameters are same as before) according to mean field theory. Here, $q = q_x$, $q_y = q_z = 0$. (b) Pair correlation function C_q for a 1D chain of $N = 60$ sites obtained by DMRG. The peak is located at $0.433\pi/a$ in both figures, which corresponds to the value $k_{F\uparrow} + k_{F\downarrow} = (N_s + N - N_p)\pi/Na$ for $N_s = 49$ and $N_p = 15$.

By fast sweeping the magnetic field (and thus the interaction) from the BCS region to the deep BEC region across a Feshbach resonance, the BCS pairs are projected onto Feshbach molecules, which can be further probed for example by time-of-flight images [13]. The bosons produced effectively reside in p band and are stable, since by Pauli blocking the filled s-band fermions will prevent the the p-wave bosons from decaying [13]. Here, we use a simple model [25, 26] to evaluate the momentum distribution of molecules after projection

$$n_{\mathbf{q}} = \sum_{\mathbf{k},\mathbf{k'}} f_{\mathbf{k}}^* f_{\mathbf{k'}} \langle S_{\mathbf{k}+\mathbf{q}/2}^\dagger P_{-\mathbf{k}+\mathbf{q}/2}^\dagger P_{-\mathbf{k'}+\mathbf{q}/2} S_{\mathbf{k'}+\mathbf{q}/2} \rangle, \quad (15)$$

where $f_{\mathbf{k}}$ is the molecular wave function, and the correlation function can be evaluated within mean field theory [26]. For fast sweeps, the molecular size is small compared to lattice constant and its wave function can be approximated by a delta function in real space (a constant $\sqrt{1/N}$ in momentum space). By this assumption, n_q is the same quantity as C_q in Eq. (6). Figure 5(a) shows the n_q of p-wave Feshbach molecules and a peak is located at $0.433\pi/a$. Figure 5(b) shows C_q from Eq. (6), based on the DMRG results shown in Fig. 1(b).The time-of-flight experiment is predicted to distribute peaks corresponding to that in Fig. 5. Note that for the 1D problem (Fig. 5(b)), the delta-function peak is replaced by a cusp characteristic of power law due to the lack of long range order.

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